Virtual Nanoscience Laboratory: A Tool for the Mesoscale Simulation of Nanomaterials

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On December 3, 2003, the President signed the 21st Century Nanotechnology Research and Development Act, assigning $3.7 billion dollars for FY 2005–2008 to nanotechnology R&D. This bipartisan legislation, that passed the House and the Senate with overwhelming support, recognizes the need to focus the efforts of the scientific community to make progress in the development and understanding of nanoscience.

The emerging fields of nanoscale science, engineering, and technology — the ability to work at the molecular level, atom by atom, to create large structures with fundamentally new properties and functions — are leading to unprecedented understanding and control over the basic building blocks and properties of all natural and man-made things. The word technological revolution is often used in relation with the current research and development of nanotechnologies.

An enumeration of the areas interested by nanotechnology would resemble the phone book. For the Laboratory and DOE, nanoscience is not only important for its relevance to strategic science but also for the interest towards material science applied to stockpile stewardship. Furthermore, chemical and biological threats can be hidden within new developments in nanotechnologies. It should be emphasized that indeed DOE is one of the five agencies involved in the 21st Century Nanotechnology Research and Development Act.

We have recently initiated an international collaboration with the Polytechnic University of Turin in Italy and with the Sumitomo Company in Japan, to develop a new computer simulation capability for nanoscale processes. We are developing the Virtual Nanoscience Laboratory that can provide the nanoscience community with a tool for the simulation of processes that live in the cross-linked area covered by atomistic, nano, and bulk scales. Nanomaterials are by definition materials where the intrinsic scales link at the lower end the atom scale and at the higher end the macroscopic continuum scale. Neither approach is sufficient: too many atoms are involved to make a pure atomistic model viable and too many structures and processes at the nano and subnano scale are important to simply resort to continuum models. New theories and new numerical approaches have to be devised.

To address the presence of such diverse time and length scales and the multiplicity of physical processes, we have proposed a new approach [1]. We bridge the gap by interlinking three numerical schemes: Molecular Dynamics (MD) for the smallest (atomistic) scales, Particle-In-Cell (PIC) for the intermediate (nano) scales and finite volume (FV) methods for the largest (bulk) scales. The key ingredient of the algorithm is the use of an intermediate scale between the nanoscale object and the atoms that compose it: we called it *cluster* (of atoms). With the use of computational clusters we designed an efficient scheme that allows us to bridge such diverse scales that range over several orders of magnitude.

A crucial innovation of the Virtual Nanoscience Laboratory is the use of a software architecture based on the Java language. This feature provides two advantages. The first is the ability to achieve remarkable parallel performances thanks to the innovations introduced in the object-oriented

Java programming environment [2]. The second is to make the Virtual Nanoscience Laboratory available to anyone over the Web, the strongest feature of the Java language. We remark that our effort in the development of a new high-performance scientific computing paradigm based on the Java language has been awarded the R&D 100 prize in 2005 with the CartaBlanca team.

To illustrate the capability of the Virtual Nanoscience Laboratory, we present results of a recent application of this approach to the simulation of nanoparticles formation in self-propagating high-temperature synthesis process (SHS) reactors [1]. The SHS is a promising method employed for the synthesis of many advanced nanomaterials, such as ceramics, intermetallics, composites, starting from a powders mixture formed by compacting micron-sized pellets. The SHS exploits the ability of certain material mixtures in producing high exothermic and self-sustaining reactions once ignited locally or uniformly. Ignition can be initiated by a laser, by induction, by resistance, by radiant heat, or by a spark source. The exothermal reaction increases the temperature rapidly producing the combustion of the micron-sized particles and the formation of much smaller non-sized particles.

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[1] G. Zuccaro, et al., *Comput. Phys. Comm.* **162**, 89 (2004).
[2] S. Markidis, et al., *Concurrency and Computation: Practice and Experience* **17**, 821 (2005).

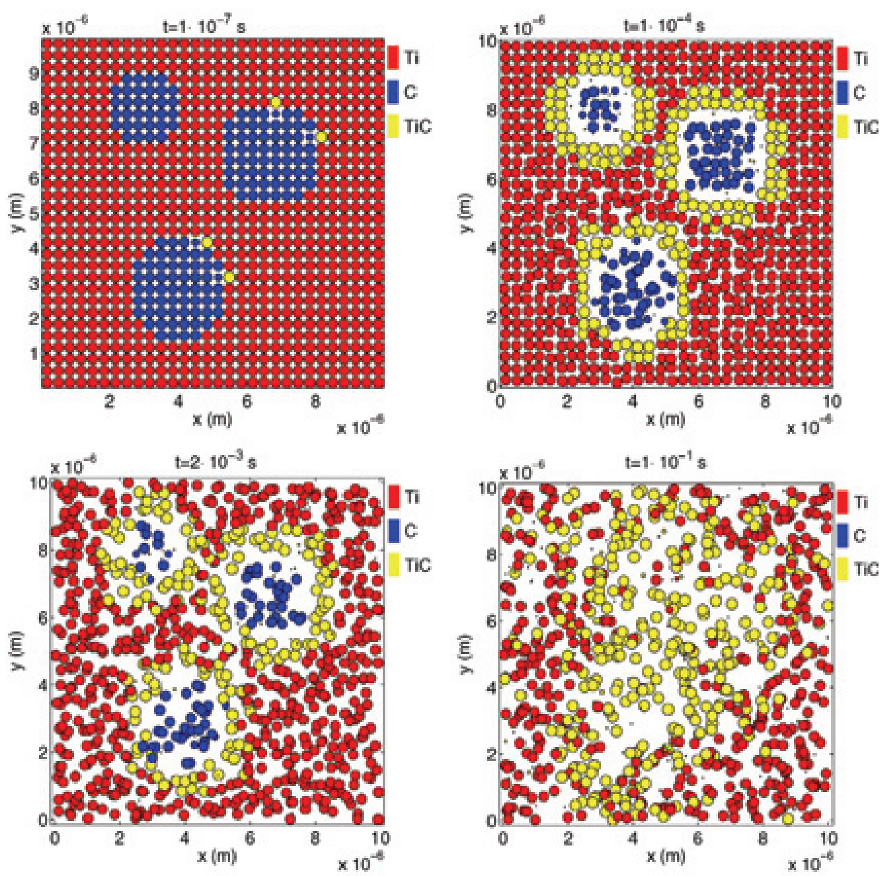

Fig. 1. ***Evolution of the SHS process, showing the disintegration of the carbon microparticles (blue) and the formation of the TiC nanoparticles (yellow). The reacting Ti is in red.***